

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101823\
 Data File : BF135861.D
 Acq On : 18 Oct 2023 22:27
 Operator : CG\JU
 Sample : 04882-02
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VNJ-218

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135861.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.199	15	19	27	rVB	38358	59166	1.79%	0.237%
2	2.787	114	119	129	rBV	40514	70528	2.13%	0.282%
3	4.334	378	382	401	rBV	996159	1282256	38.80%	5.132%
4	4.981	485	492	520	rVB	1916974	3304963	100.00%	13.228%
5	5.387	557	561	588	rBV	2562638	2751007	83.24%	11.011%
6	5.763	621	625	639	rVB	98251	111461	3.37%	0.446%
7	6.398	729	733	759	rBV	2577085	2767118	83.73%	11.075%
8	6.740	788	791	802	rVB	557948	510841	15.46%	2.045%
9	7.310	884	888	901	rBV	1984331	1783013	53.95%	7.137%
10	8.016	1005	1008	1026	rVB	813036	705256	21.34%	2.823%
11	9.098	1188	1192	1195	rBV	3523349	2990958	90.50%	11.971%
12	9.210	1208	1211	1216	rBV	60599	67844	2.05%	0.272%
13	9.775	1303	1307	1319	rBV	852735	702008	21.24%	2.810%
14	10.575	1439	1443	1458	rBV	1900476	1829770	55.36%	7.324%
15	11.269	1558	1561	1564	rBV	796694	735180	22.24%	2.943%
16	11.298	1564	1566	1572	rVB	159796	152352	4.61%	0.610%
17	11.780	1645	1648	1650	rBV	45323	44489	1.35%	0.178%
18	11.804	1650	1652	1660	rVV2	428236	456658	13.82%	1.828%
19	11.886	1664	1666	1669	rBV	44828	43556	1.32%	0.174%
20	12.127	1704	1707	1713	rVB5	25391	35993	1.09%	0.144%
21	12.333	1739	1742	1744	rBV	47935	40853	1.24%	0.164%
22	12.498	1766	1770	1774	rBV	252716	239979	7.26%	0.961%
23	12.592	1784	1786	1794	rBV	109901	143629	4.35%	0.575%
24	12.727	1804	1809	1813	rBV	216871	226124	6.84%	0.905%
25	12.869	1829	1833	1836	rBV	2507013	2443689	73.94%	9.781%
26	13.704	1971	1975	1979	rVB4	23084	39984	1.21%	0.160%
27	13.857	1994	2001	2007	rBV8	28976	83298	2.52%	0.333%
28	13.939	2011	2015	2018	rVV	425797	445991	13.49%	1.785%
29	13.963	2018	2019	2023	rVB	58767	54565	1.65%	0.218%
30	14.398	2090	2093	2097	rBV4	28427	37340	1.13%	0.149%
31	14.504	2105	2111	2112	rBV3	27894	47990	1.45%	0.192%
32	14.557	2117	2120	2124	rBV2	62675	74518	2.25%	0.298%
33	14.992	2190	2194	2197	rBV	49881	74220	2.25%	0.297%
34	15.298	2242	2246	2251	rVB	35288	41898	1.27%	0.168%
35	15.363	2254	2257	2261	rVB	35997	37492	1.13%	0.150%
36	15.415	2262	2266	2273	rBV	346573	447445	13.54%	1.791%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.839	2336	2338	2345	rVB2	27117	37096	1.12%	0.148%
38	16.945	2521	2526	2534	rVB3	33016	63667	1.93%	0.255%

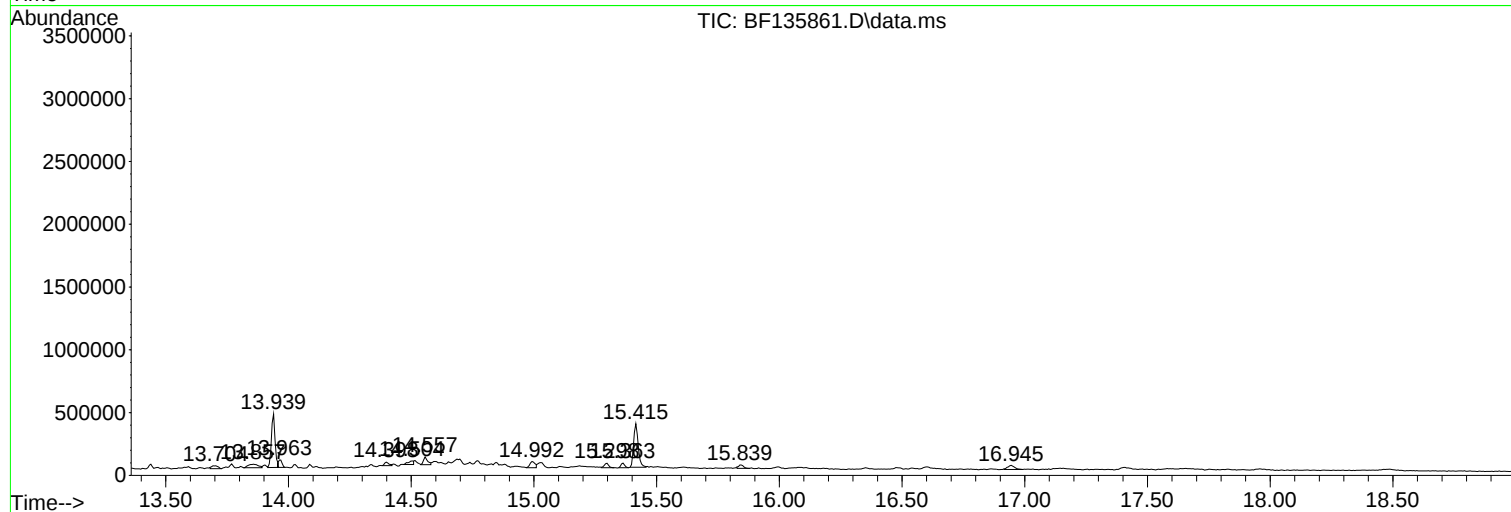
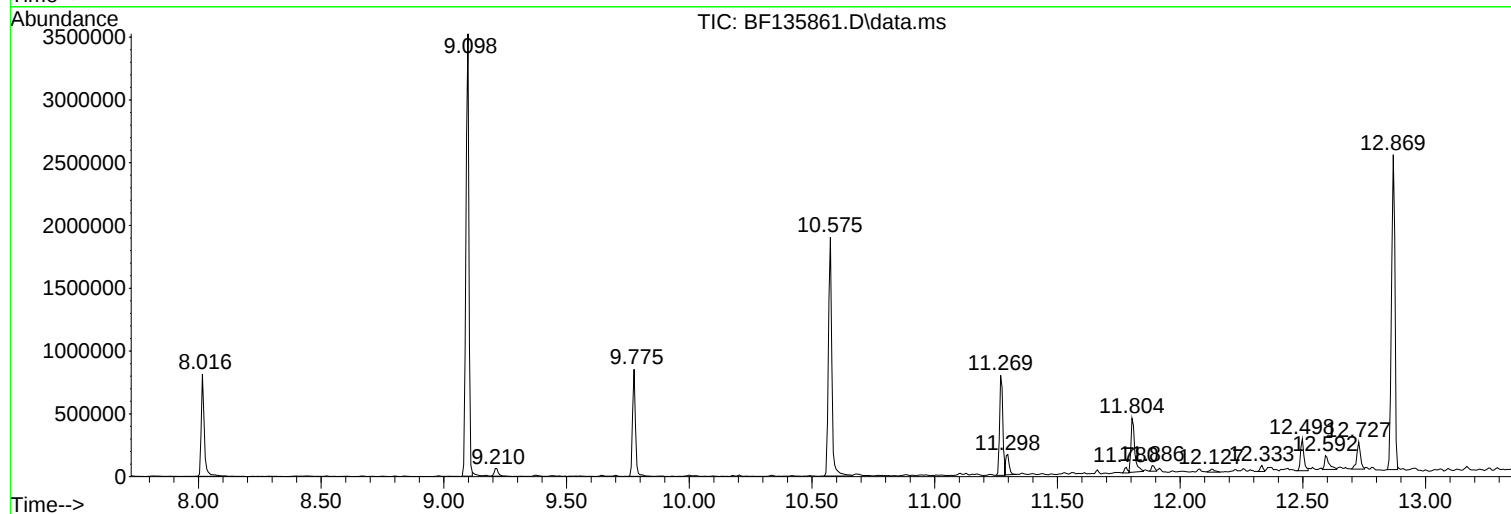
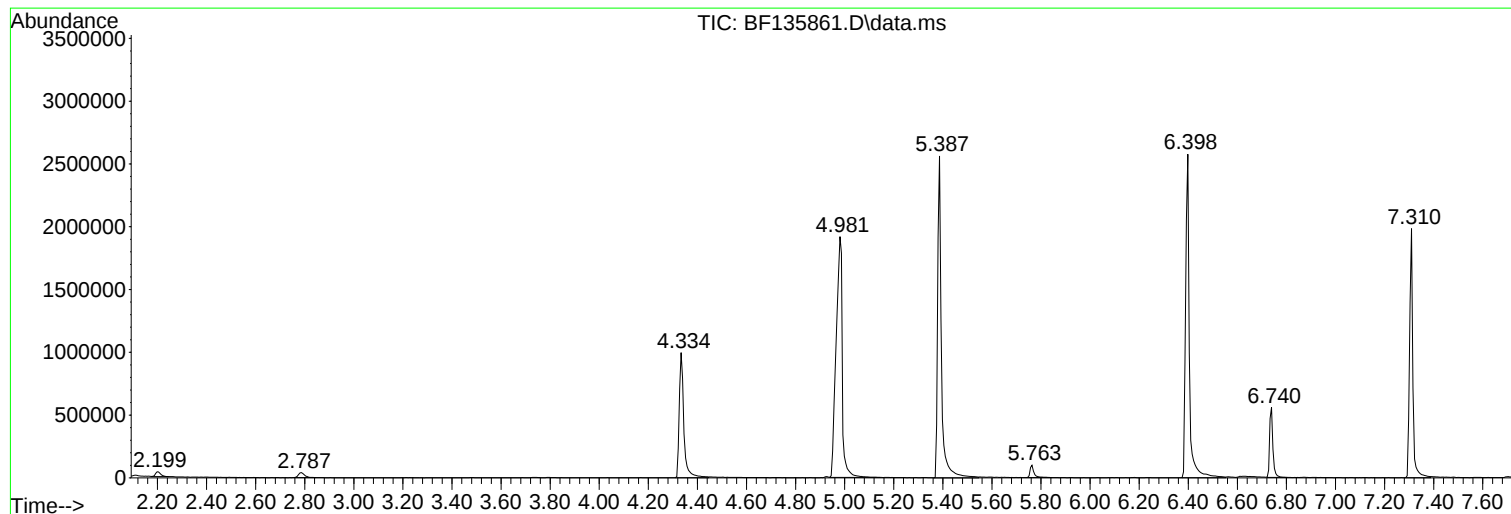
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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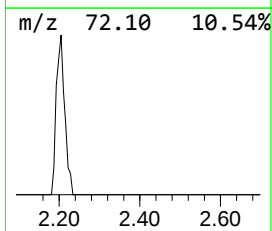
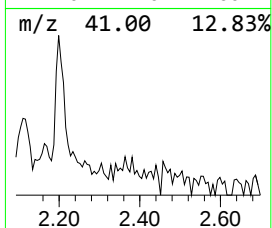
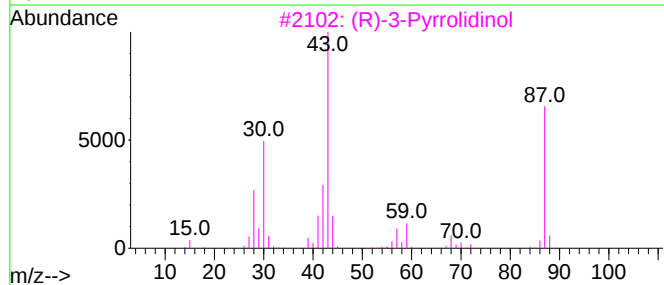
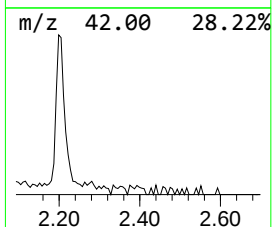
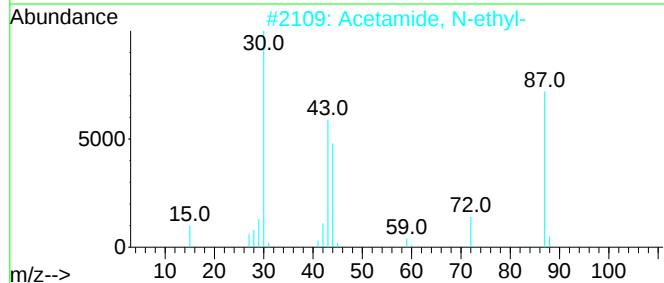
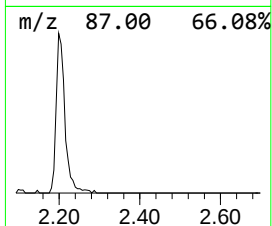
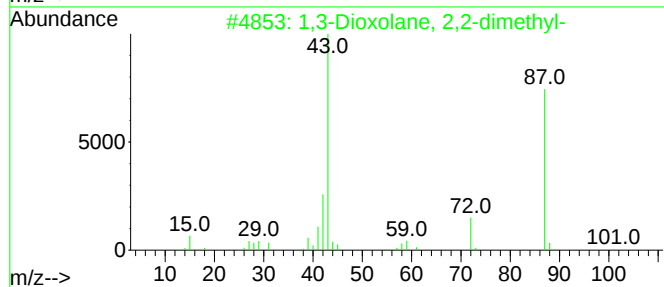
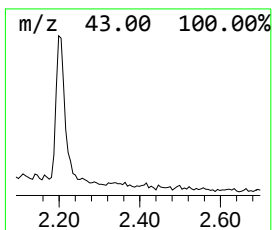
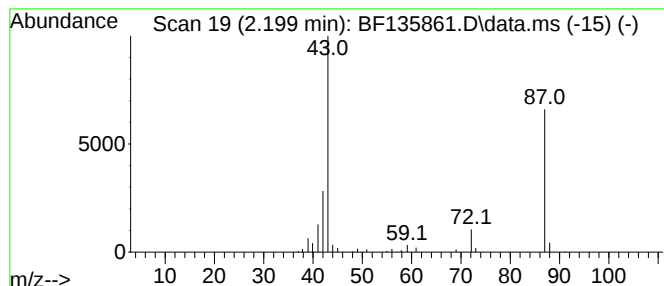
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 1,3-Dioxolane, 2,2-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.199	2.32 ng	59166	1,4-Dichlorobenzene-d4	6.740

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane, 2,2-dimethyl-	102	C5H10O2	002916-31-6	64
2			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	40
3			(R)-3-Pyrrolidinol	87	C4H9NO	002799-21-5	39
4			Ethanol, 2,2'-oxybis-, diacetate	190	C8H14O5	000628-68-2	38
5			2-Propanone, O-methyloxime	87	C4H9NO	003376-35-0	37



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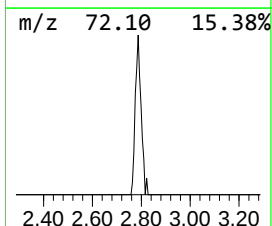
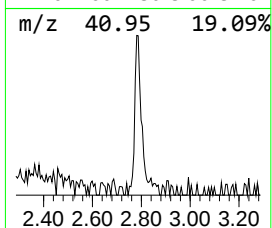
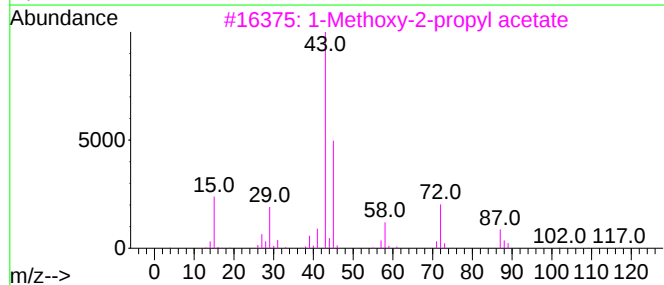
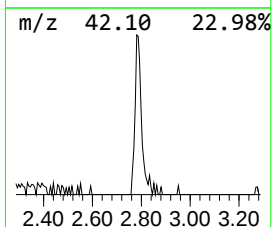
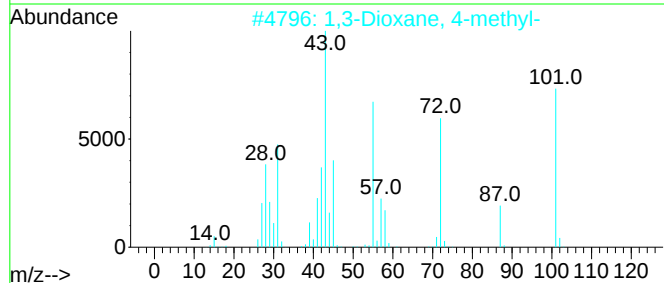
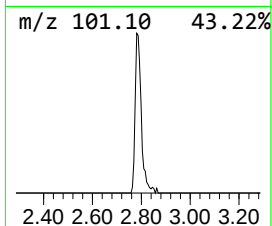
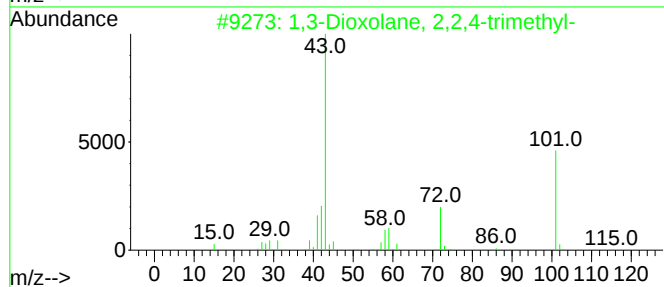
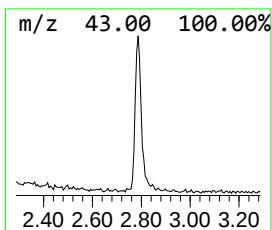
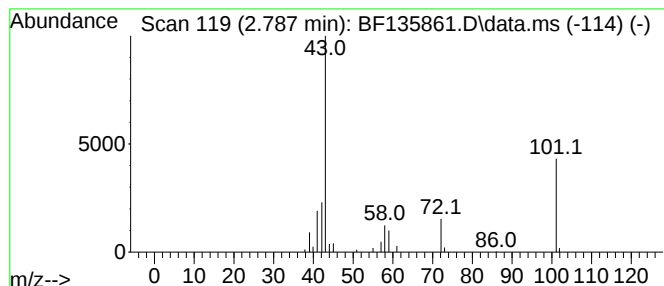
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 1,3-Dioxolane, 2,2,4-trimet... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.787	2.76 ng	70528	1,4-Dichlorobenzene-d4	6.740

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,3-Dioxolane, 2,2,4-trimethyl-	116	C6H12O2	001193-11-9	78
2		1,3-Dioxane, 4-methyl-	102	C5H10O2	001120-97-4	36
3		1-Methoxy-2-propyl acetate	132	C6H12O3	000108-65-6	12
4		2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	10
5		Butane	58	C4H10	000106-97-8	9



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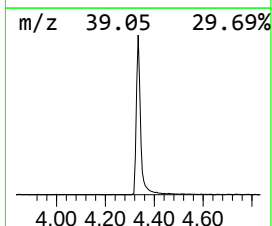
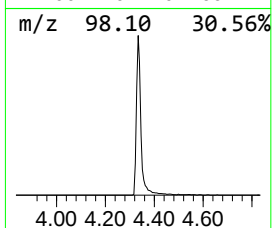
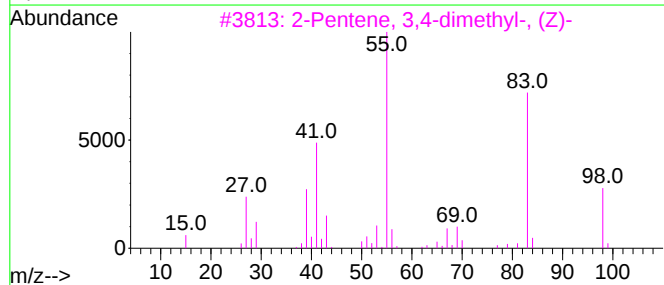
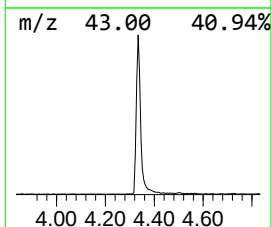
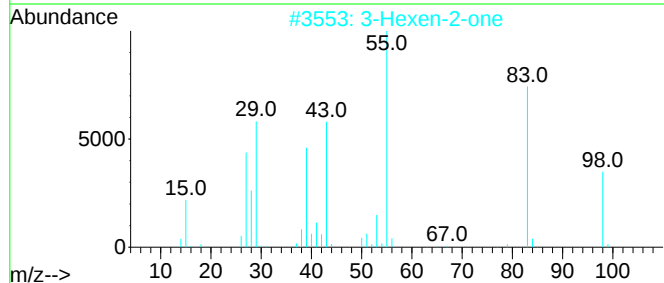
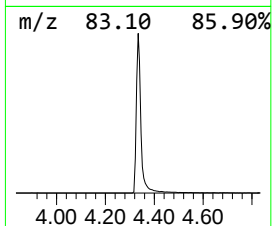
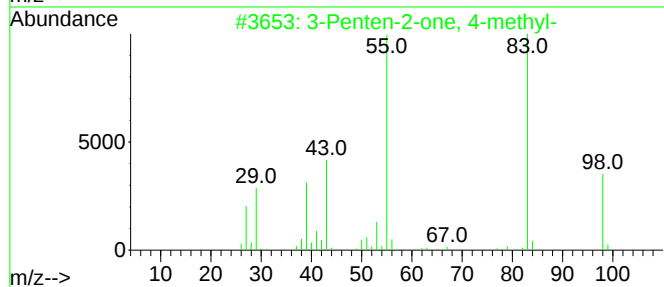
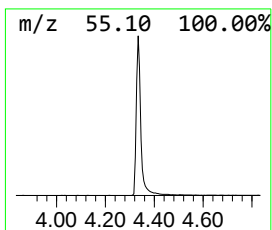
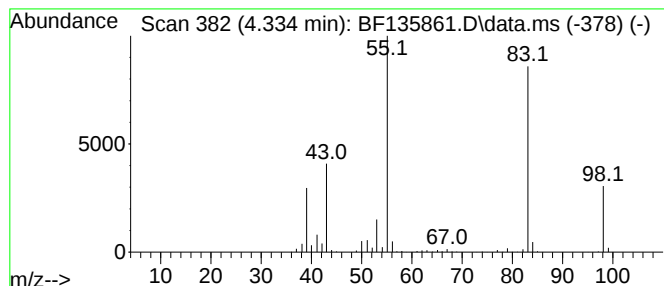
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 3-Penten-2-one, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.334	50.20 ng	1282260	1,4-Dichlorobenzene-d4	6.740

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2			3-Hexen-2-one	98	C6H10O	000763-93-9	91
3			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
4			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	72
5			2-Pentene, 3,4-dimethyl-	98	C7H14	024910-63-2	72



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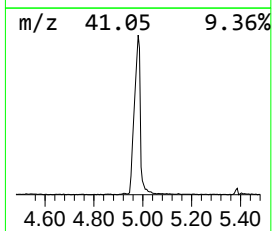
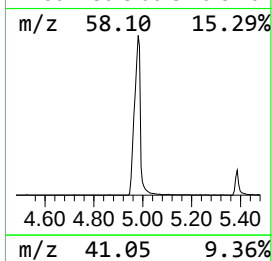
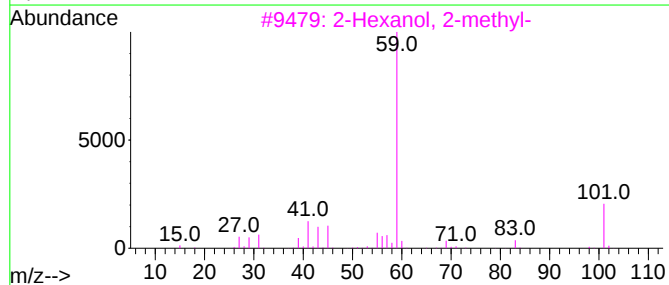
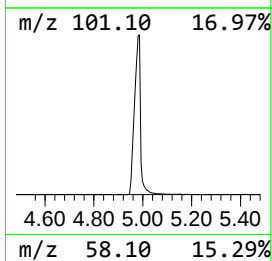
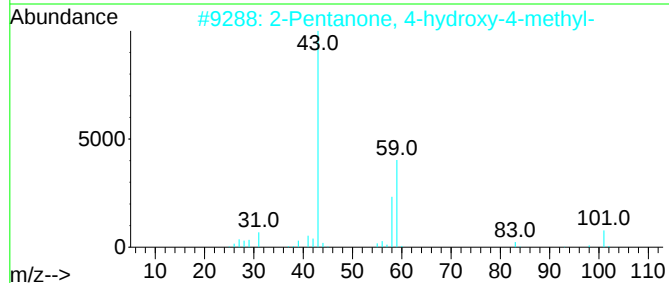
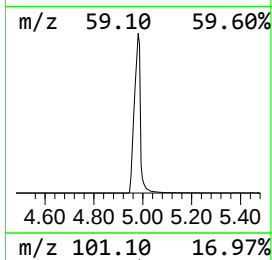
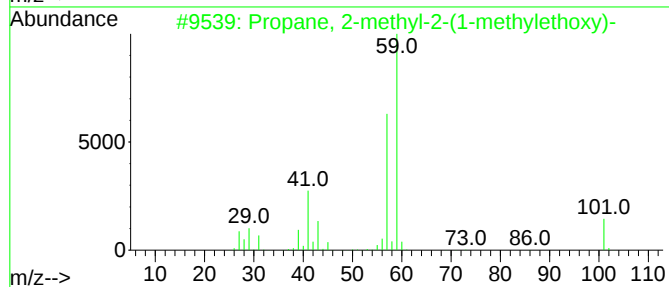
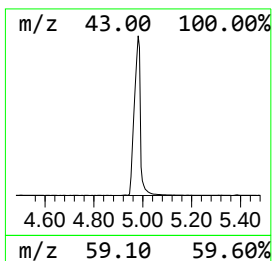
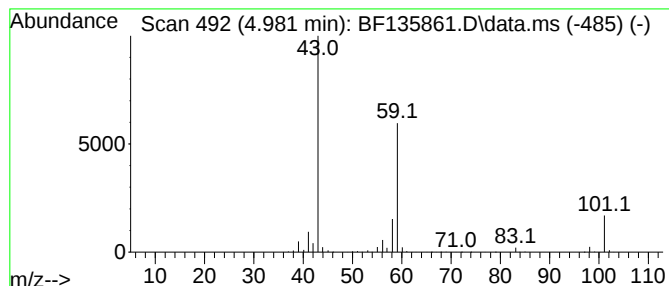
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Propane, 2-methyl-2-(1-meth... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.981	129.39 ng	3304960	1,4-Dichlorobenzene-d4	6.740

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
2			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32



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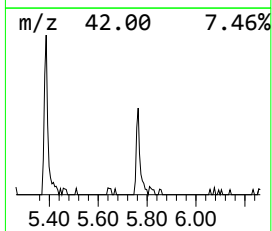
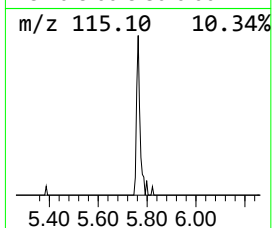
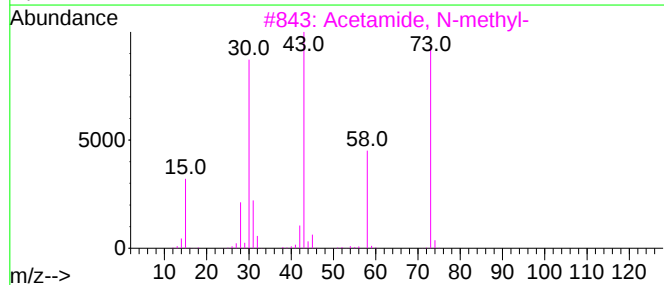
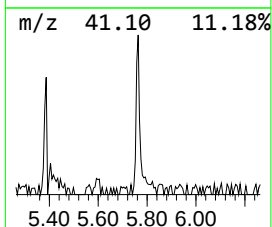
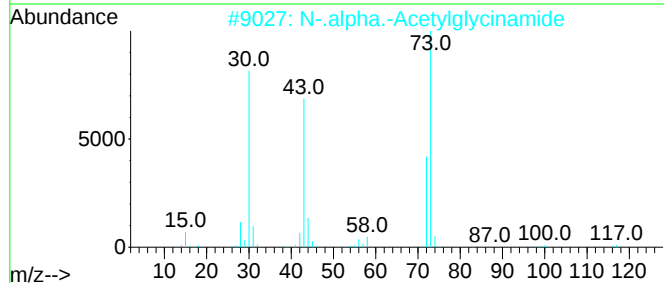
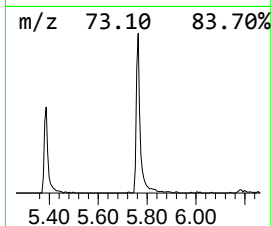
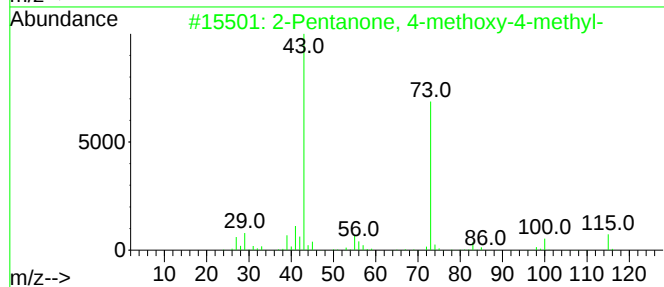
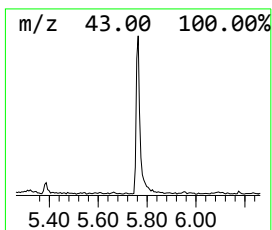
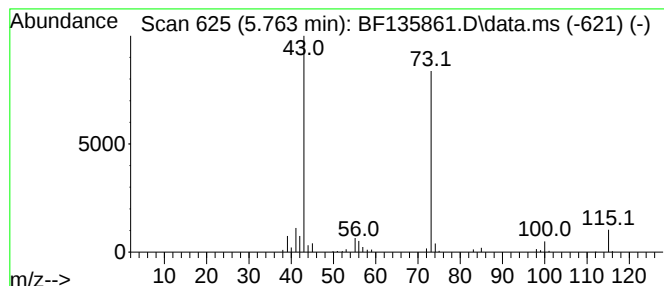
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 2-Pentanone, 4-methoxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.763	4.36 ng	111461	1,4-Dichlorobenzene-d4	6.740

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2			N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	38
3			Acetamide, N-methyl-	73	C3H7NO	000079-16-3	32
4			1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	25
5			3,6-Heptanedione	128	C7H12O2	001703-51-1	17



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101823\
Data File : BF135861.D
Acq On : 18 Oct 2023 22:27
Operator : CG\JU
Sample : 04882-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-218

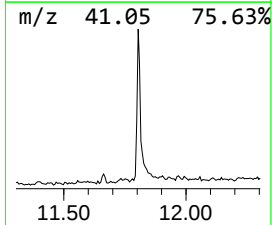
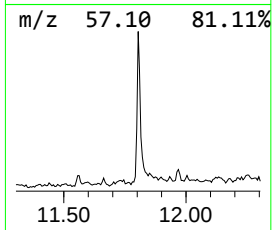
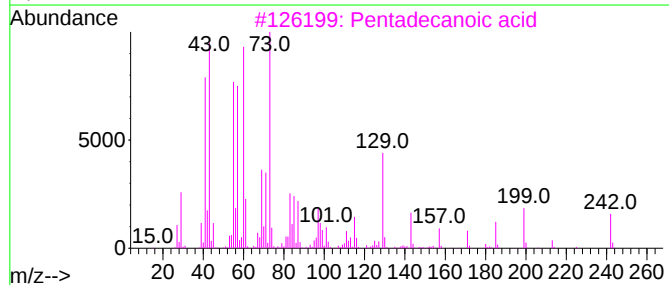
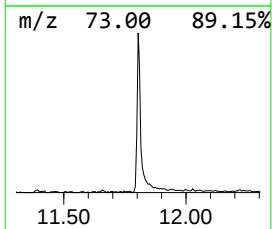
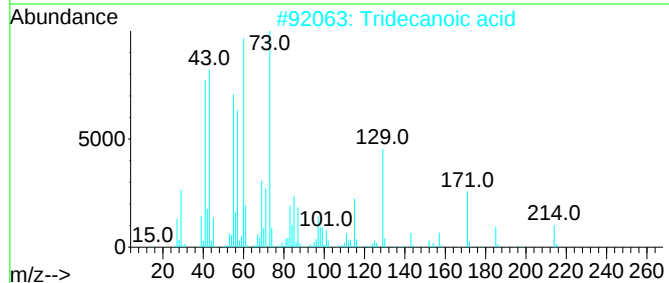
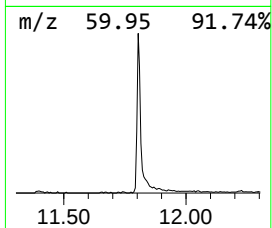
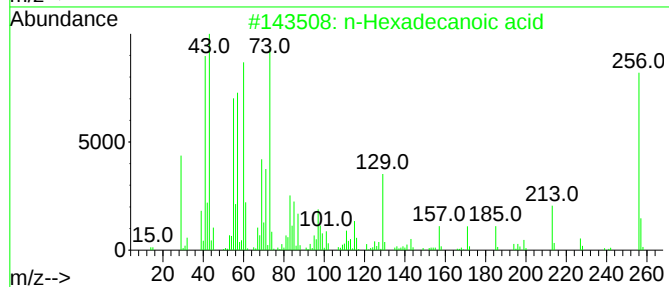
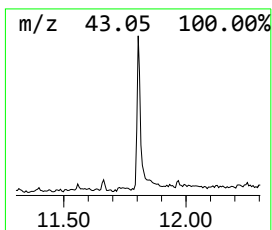
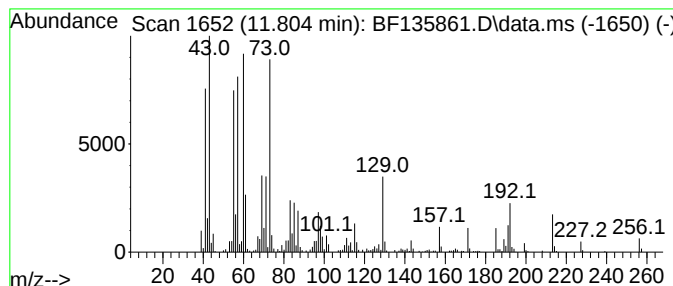
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.804	12.42 ng	456658	Phenanthrene-d10	11.269

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tridecanoic acid	214	C13H26O2	000638-53-9	93
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	59
5		Octanoic acid	144	C8H16O2	000124-07-2	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101823\
Data File : BF135861.D
Acq On : 18 Oct 2023 22:27
Operator : CG\JU
Sample : 04882-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-218

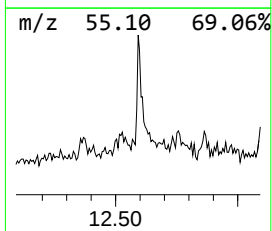
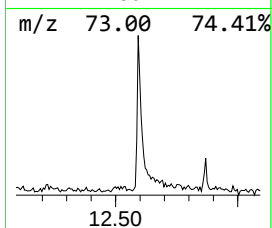
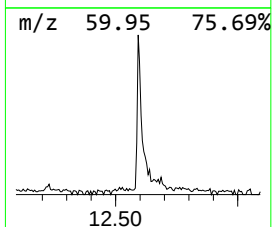
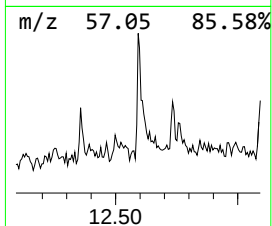
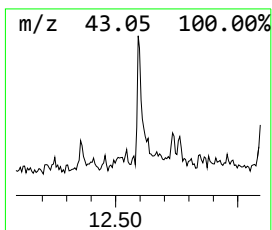
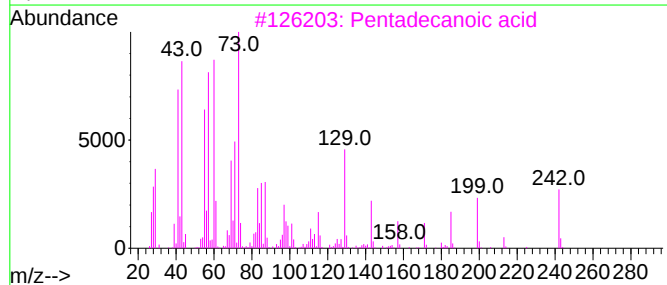
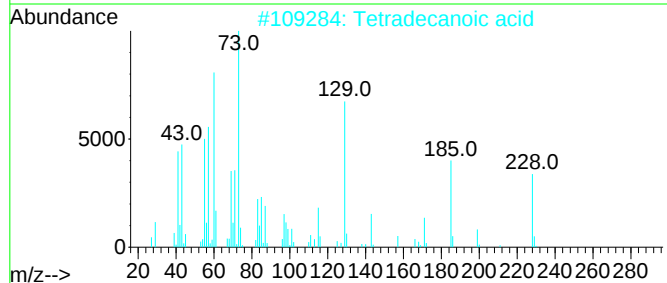
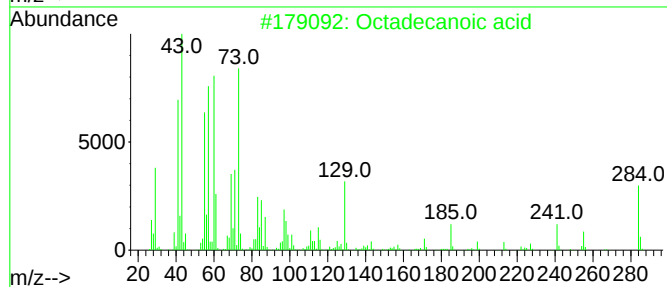
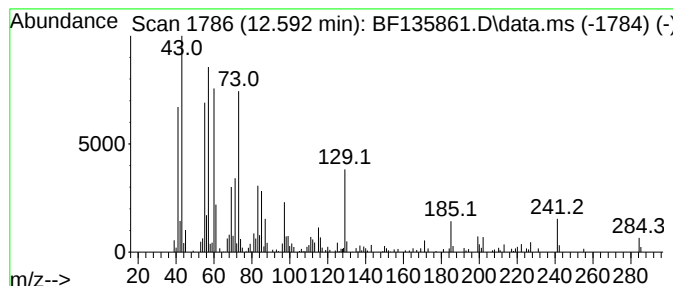
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.592	3.91 ng	143629	Phenanthrene-d10	11.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	76
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	59
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	52
4			n-Decanoic acid	172	C10H20O2	000334-48-5	50
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101823\
Data File : BF135861.D
Acq On : 18 Oct 2023 22:27
Operator : CG\JU
Sample : 04882-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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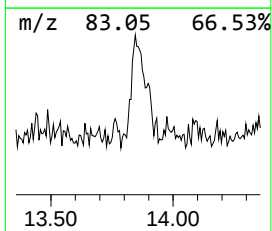
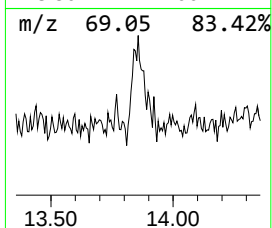
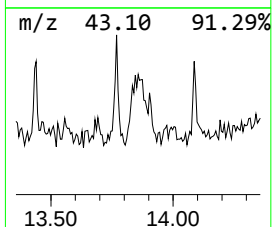
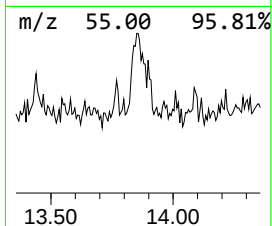
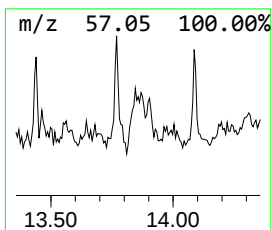
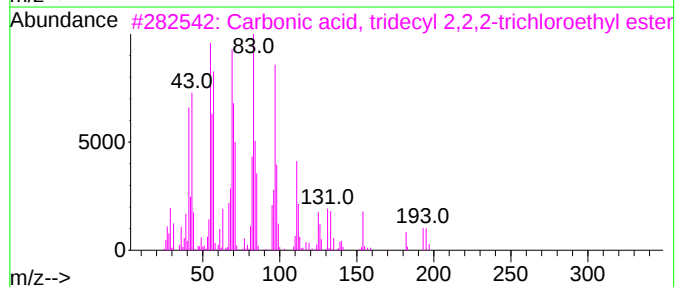
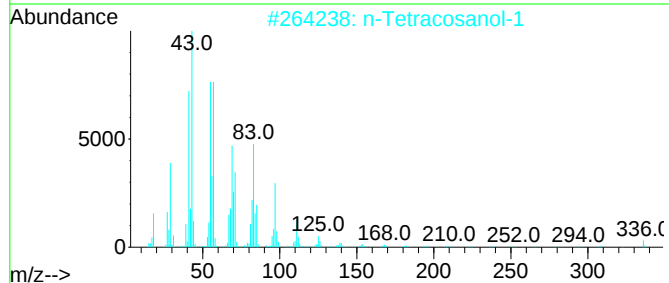
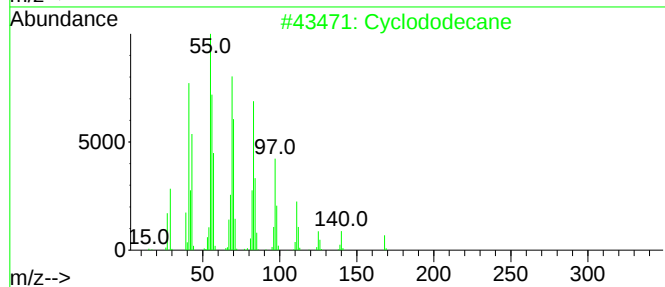
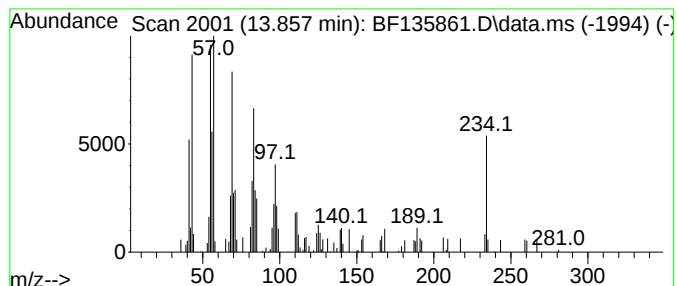
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Cyclododecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.857	3.74 ng	83298	Chrysene-d12	13.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclododecane	168	C12H24	000294-62-2	89
2			n-Tetracosanol-1	354	C24H50O	000506-51-4	74
3			Carbonic acid, tridecyl 2,2,2-tr...	374	C16H29Cl3O3	1000314-55-9	72
4			Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	68
5			Cyclotetradecane	196	C14H28	000295-17-0	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101823\
Data File : BF135861.D
Acq On : 18 Oct 2023 22:27
Operator : CG\JU
Sample : 04882-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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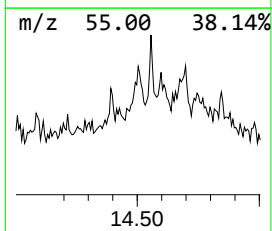
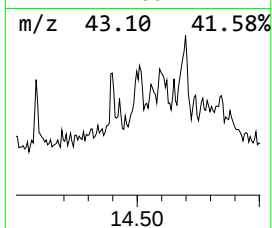
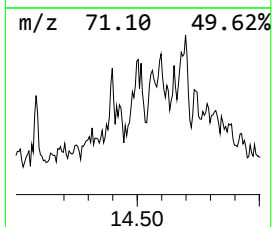
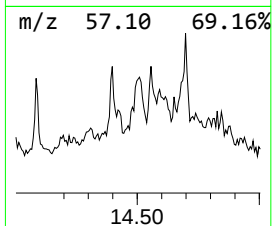
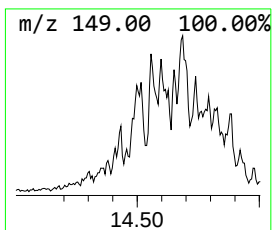
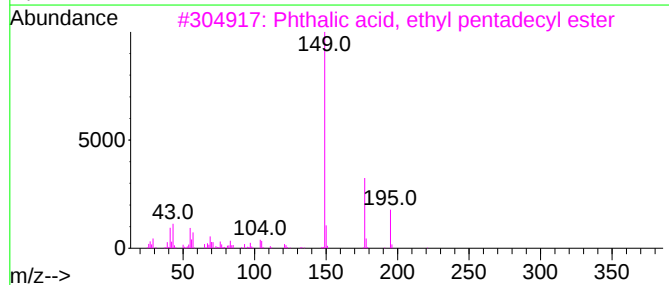
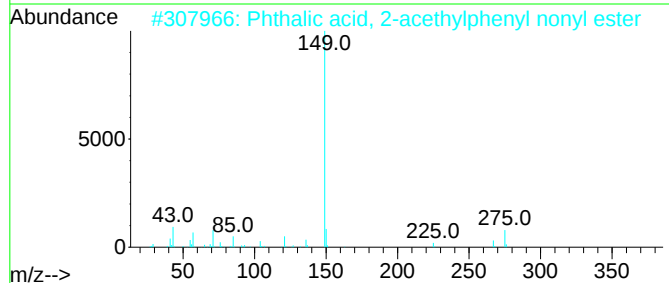
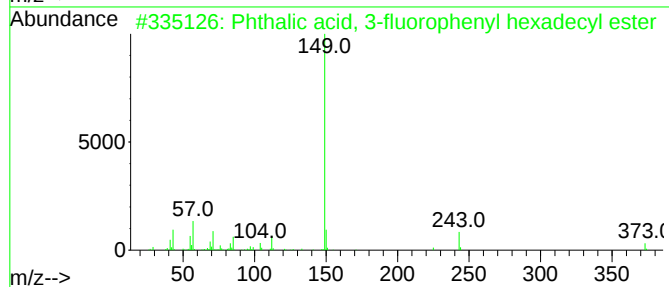
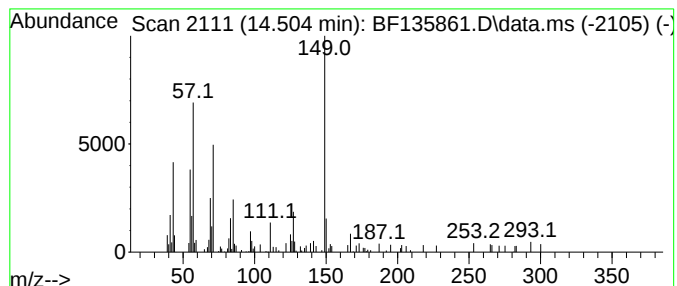
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Phthalic acid, 3-fluorophen... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.504	2.15 ng	47990	Chrysene-d12	13.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phthalic acid, 3-fluorophenyl he...	484	C30H41FO4	1000356-66-4	64
2			Phthalic acid, 2-acetylphenyl n...	410	C25H30O5	1000315-82-0	59
3			Phthalic acid, ethyl pentadecyl ...	404	C25H40O4	1000308-93-3	38
4			Phthalic acid, butyl 1-cyclopent...	318	C19H26O4	1010309-88-5	38
5			Phthalic acid, ethyl tetradecyl ...	390	C24H38O4	1000309-00-5	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101823\
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Sample : 04882-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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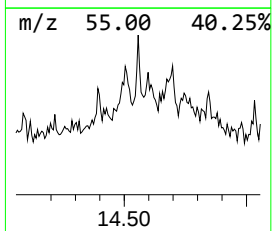
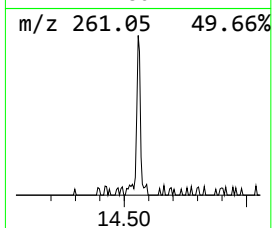
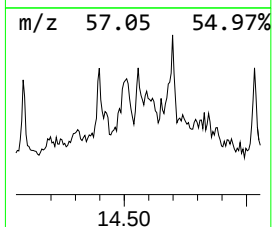
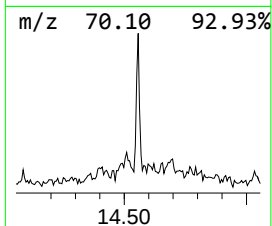
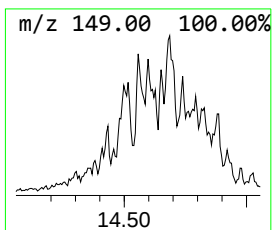
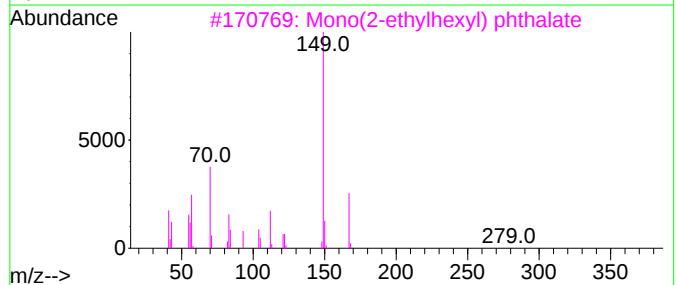
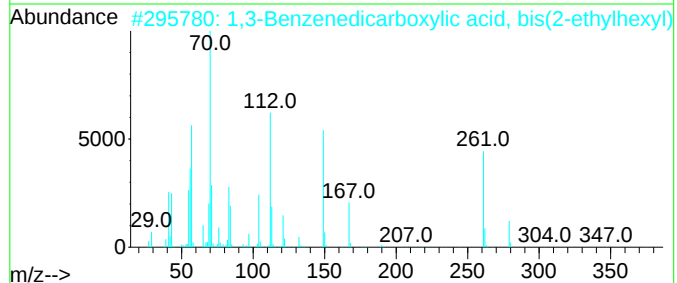
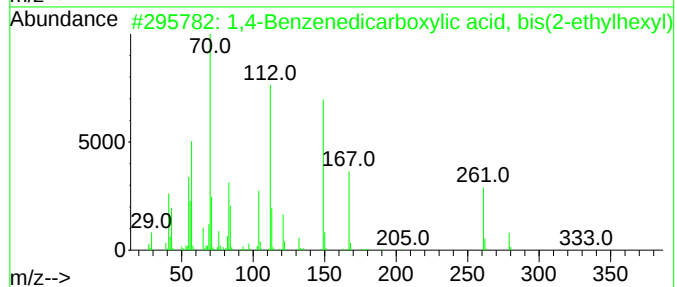
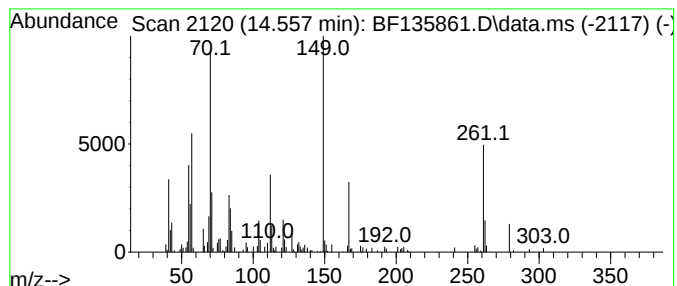
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 unknown14.557 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.557	3.34 ng	74518	Chrysene-d12	13.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	43
2			1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	38
3			Mono(2-ethylhexyl) phthalate	278	C16H22O4	004376-20-9	32
4			Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000383-13-3	27
5			2-Heptene, 3-methyl-	112	C8H16	003404-75-9	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101823\
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Operator : CG\JU
Sample : 04882-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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1,3-Dioxolane, ...	2.787	2.8	ng	70528	1	6.740	510841	20.0
3-Penten-2-one,...	4.334	50.2	ng	1282260	1	6.740	510841	20.0
Propane, 2-meth...	4.981	129.4	ng	3304960	1	6.740	510841	20.0
2-Pentanone, 4-...	5.763	4.4	ng	111461	1	6.740	510841	20.0
n-Hexadecanoic ...	11.804	12.4	ng	456658	4	11.269	735180	20.0
Octadecanoic acid	12.592	3.9	ng	143629	4	11.269	735180	20.0
Cyclododecane	13.857	3.7	ng	83298	5	13.939	445991	20.0
Phthalic acid, ...	14.504	2.1	ng	47990	5	13.939	445991	20.0
unknown14.557	14.557	3.3	ng	74518	5	13.939	445991	20.0